Malonic acid, 3,3-dimethylbut-2-yl isohexyl ester

Inchi: InChI=1S/C15H28O4/c1-11(2)8-7-9-18-13(16)10-14(17)19-12(3)15(4,5)6/h11-12H,7-10H

InchiKey: QAVARSAJQSAKET-UHFFFAOYSA-N

Formula: C15H28O4

SMILES: CC(C)CCCOC(=O)CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-394.46	kJ/mol	Joback Method
hf	-861.84	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.334		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	691.07	K	Joback Method
tc	878.32	K	Joback Method
tf	375.55	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.58	J/mol×K	691.07	Joback Method
cpg	697.58	J/mol×K	722.28	Joback Method
cpg	713.66	J/mol×K	753.49	Joback Method
cpg	728.85	J/mol×K	784.70	Joback Method
cpg	743.16	J/mol×K	815.90	Joback Method
cpg	756.61	J/mol×K	847.11	Joback Method
cpg	769.22	J/mol×K	878.32	Joback Method
dvisc	0.0022315	Pa×s	375.55	Joback Method

dvisc	0.0009002	Pa×s	428.14	Joback Method
dvisc	0.0004430	Pa×s	480.72	Joback Method
dvisc	0.0002507	Pa×s	533.31	Joback Method
dvisc	0.0001571	Pa×s	585.90	Joback Method
dvisc	0.0001064	Pa×s	638.48	Joback Method
dvisc	0.0000764	Pa×s	691.07	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume